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SSC-DFTB parameterization of Pd and TiO_2 systems

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Abstract :

The self-consistent-charge density functional tight binding (SCC-DFTB) approach has been used to describe large scale systems with less computational cost than the density functional theory method [1]. DFTB+ has been used to develop a set of SCC-DFTB parameters for Pd-Pd and Ti-X (X = Ti, O) also considering O-O atomic pairs of elements. The SCC-DFTB parameterization has been performed to describe periodic systems Pd and TiO_2 respectively. It was found that the structural properties obtained from the parameters were good. Comparison to the lattice parameter obtained from geometry optimization for bulk Pd and TiO_2 was found to be within 0.1% with the available literature data [2-4]. The SSC-DFTB+ set of parameters obtained within this study have also been successful in describing the electronic properties of TiO_2. The calculated electronic band structure of TiO_2 yielded an energy band gap of 3.21 eV, in excellent agreement with the experimental value of 3.2 eV [5]. References [1] A. F. Oliveira, G. Seitfert, T. Heine, H. A Duarte, J. Braz. Chem. Soc. 20 (2009) 1193[2] D. Schebarchov and S. Hendy, Phys. Rev. B 73 (2006), 121402[3] M. Horn, C.F. Schwerdtfeger and E.P.Z. Meagher, Kristallogr. 136 (3-4) (1972) 273[4] G. Dolgonos, B. Aradi, N.H. Moreira and T. Frauenheim, J. Chem. Theory Comput. 6 (2010) 266[5] F. Labat, P. Baranek, C. Domain, C. Minot and C. Adamo, J. Chem. Phys. 129 (2007) 154703

Award :

No

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